PhD 2021-2024 Ecole Doctorale de Chimie de Lyon

Multifunctional magnetic molecular materials with Boron-Nitrogen bonds
Synthesis and study of the magneto-structural properties

Matériaux moléculaires magnétiques multifonctionnels avec des liaisons Bore-Azote
Synthèse et étude des propriétés magnéto-structurales

Supervisors :	Dominique LUNEAU, Professor,	luneau@univ-lyon1.fr / +33(0)472-431-418
	Bérangère TOURY, Ass. Professor,	toury@univ-lyon1.fr / +33(0)472-433-612

Laboratoire des Multimatériaux et Interfaces (UMR 5615) – Université Claude Bernard Lyon 1

Keywords: inorganic chemistry; boron; nitroxide radicals; magnetism; crystallography

Contexte: Some coordination complexes may acquire a persistent magnetization in the manner of classical magnets. Unlike the latter, this is not a property of the solid state but of the single molecule (Single Molecule Magnets: SMM) [1]. To show this behavior, a complex must have a high magnetic moment with a strong magnetic anisotropy. SMMs generate a strong international competition for their potentialities related to information processing. They are indeed molecular-sized memory units (bit) with prospects in molecular spintronics or quantum computing [2].

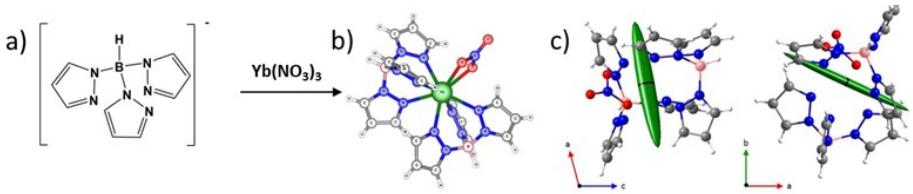

Fig. 1

Objectives: Following previous work (Fig. 1) [3] the objective of the PhD will be to synthesize such mono- or polynuclear systems using coordination chemistry methods with ligands containing BN bonds (scorpionates [3-4]; borazines [5]; BN-cyclohexanes [6]; Borazatruxenes [7] ...). A first step will be the synthesis of the BN bonded systems which generally require to work under an inert atmosphere. These systems will be used to complex magnetic metal ions (*3-5d or 4f*) or/and will be even functionalized with nitroxide radicals to build molecule based magnets. A special care will be dedicated to obtain all compounds in the form of single crystals. This is required for the crystal structure determination, by X-ray diffraction, of the precursors and complex systems in close relation with the synthesis work and the study of magnetic properties. One concern will be to understand the magneto-structural relationships in these systems. The project relies on the strong and complementary skills within the host team (CIMP) and the *Laboratoire des Multimatériaux et Interfaces* (LMI) in coordination and boron chemistries, crystallography and molecular magnetism and on a national and international collaboration network [8-9]. Synthesis work, crystallographic studies and systematic magnetic measurements will be carried out at the LMI. Charge density and spin density mapping using high resolution X-ray diffraction and neutron diffraction will be considered for the most interesting systems in the frame of collaboration.

Situation: Interdisciplinary basic research that aims applications combining chemistry, materials and physic.

Requested: Solid curriculum in chemistry with ability to apprehend physical phenomena. Strong motivation for inorganic synthesis, crystallography and magnetic studies. Ability to work independently

Skills to be developed: Synthesis under an inert atmosphere using Schlenk and glove box techniques; crystal structure determination from X-ray diffraction and magnetic studies with SQUID magnetometer.

Bibliographie : [1] a) D. Gatteschi, R. Sessoli *Angew. Chem. Int. Ed* **2003**, 42, 268-297. (b) M. J. Giansiracusa, A. K. Kostopoulos, D. Collison, R. E. P. Winpenny and N. F. Chilton, *Chem. Commun.*, **2019**, 55, 7025-7028. (c) F. S. Guo, A. K. Bar and R. A. Layfield, *Chem. Rev.* **2019**, 119, 8479-8505. [2] (a) M. Leuenberger, N., D. Loss, *Nature* **2001**, 410, 789-793. (b) L. Bogani and W. Wernsdorfer, *Nat. Mater.* 2008, 7, 179. [3] (a) F. Guegan, J. Jung, B. Le Guennic, F. Riobe, O. Maury, B. Gillon, J. F. Jacquot, Y. Guyot, C. Morell and D. Luneau, *Inorg. Chem. Front.* **2019**, 6, 3152-3157. (b) F. Guegan, F. Riobe, O. Maury, J. Jung, B. Le Guennic, C. Morell and D. Luneau, *Inorg. Chem. Front.*, **2018**, 5, 1346-1353. [4] S. Trofimenko, *Chem. Rev.* **1993**, 93, 943-980. [5] (a) J. L. Chen, H. Feng, Y. M. Xie, R. B. King and H. F. Schaefer, *New J. Chem.* **2019**, 43, 4497-4505. 1. (b) S. Kervyn, O. Fenwick, F. Di Stasio, Y. S. Shin, J. Wouters, G. Accorsi, S. Osella, D. Beljonne, F. Cacialli and D. Bonifazi, *Chem. Eur. J.* **2013**, 19, 7771-7779 [6] A. Kumar, J. S. A. Ishibashi, T. N. Hooper, T. C. Mikulas, D. A. Dixon, S. Y. Liu and A. S. Weller, *Chem. Eur. J.*, **2016**, 22, 310-322. [7] S. Limberti, L. Emmett, A. Trandafir, G. Kociok-Kohn and G. D. Pantos, *Chemical Science*, 2019, 10, 9565-9570. [8] D. Luneau (ORCID: 0000-0002-1831-7693). [9] B. Toury (ORCID: 0000-0001-5889-0796).